

Methyl beta-alanate
4138-35-6 | DTXSID50194322

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 53.2 °C

Global applicability domain: Inside

Local applicability domain index: 4.47e-01

Confidence level: 5.46e-01

Nearest Neighbors from the Training Set

Image not found

Thioacetamide

Measured: 116

Predicted: 113

Image not found

Ethanamine, 2,2-diethoxy-

Measured: -78.0

Predicted: -53.9

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N-Methylacetamide

Measured: 28.0

Predicted: 37.6

Image not found

Propanamide, 2-methyl-

Measured: 128

Predicted: 122

Image not found

Propanamide

Measured: 81.3

Predicted: 92.6